Abstract Submitted
for the OSS17 Meeting of
The American Physical Society

**Instability of Non-Ergodic Effects in Anharmonic Atomic Chains: Singular Dependence** CHRISTOPHER WATENPOOL, DONALD PRIOUR, Youngstown State University — We use large scale molecular dynamics simulations to calculate equilibration times in anharmonic chains, with the anharmonicity being a quartic term in the interaction potential. In the latter case, where the system is thermally insulated from its environment, equilibration via internal dynamics is hampered, characterized by non-ergodic effects such as long term oscillations. We relax the isolation, allowing the ends of the chain to couple to external heat baths (implemented with the Langevin technique). In our calculations we quantify equilibration times using the decay exponents of the energy stored in the fundamental mode or the attainment of a specified threshold in a measure of mode engagement, finding in the thermodynamic limit a scaling form $\tau = AN^{\eta}$ with $\eta$ being a scaling exponent. Whether the anharmonicity is weak or strong, we find equilibration to be significantly hastened by the heat bath coupling. Moreover, we find singular behavior, in the sense that any finite coupling to the terminal heat baths leads not only to the same scaling exponent $\tau$, but also the same pre-factor $A$. Since a system realized in the experiment would be difficult to fully isolate suggesting that non-ergodic effects may be difficult to observe in practice in bulk systems.

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Date submitted: 07 Apr 2017 Electronic form version 1.4